

6-(2-Methylbutyryloxy)-hyoscyamine

Inchi: InChI=1S/C22H31NO5/c1-4-14(2)21(25)28-20-11-16-10-17(12-19(20)23(16)3)27-22(26)
InchiKey: ATYKKAWWFYZZJF-QHGFLKOESA-N
Formula: C22H31NO5
SMILES: CCC(C)C(=O)OC1CC2CC(OC(=O)C(CO)c3ccccc3)CC1N2C
Mol. weight [g/mol]: 389.49

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.65 | | Crippen Method |
| logp | 2.499 | | Crippen Method |
| mcvol | 306.090 | ml/mol | McGowan Method |
| rinpol | 2539.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R421720&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/41-641-4/6-2-Methylbutyryloxy-hyoscyamine.pdf>

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